

# Phase ordering in 3d disordered systems

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We study numerically the phase-ordering kinetics of the site-diluted and bond-diluted Ising models after a quench from an infinite to a low temperature. We show that the speed of growth of the ordered domain's size is non-monotonous with respect to the amount of dilution  $D$ : Starting from the pure case  $D = 0$  the system slows down when dilution is added, as it is usually expected when disorder is introduced, but only up to a certain value  $D^*$  beyond which the speed of growth raises again. We interpret this counterintuitive fact in a renormalization-group inspired framework, along the same lines proposed for the corresponding two-dimensional systems, where a similar pattern was observed.

## I. INTRODUCTION

The quench of systems, like ferromagnets or binary mixtures, to below the critical point is characterized by the formation and subsequent growth of domains. The typical feature of the phase ordering process is dynamical scaling, whereby physical properties become time-independent if lengths are measured in units of  $L$ , i.e. the typical domain size at time  $t$  [1–7]. This scaling scenario is expected to be valid also in presence of quenched disorder when it does not prevent the phase-ordering process [7, 8]. In the case of pure systems power law growth  $L \sim t^{1/z}$  is well established. Conversely, when disorder is present the nature of asymptotic growth has been much debated [9–22].

In general terms, disorder generated energy barriers bring about a slowing down of the coarsening process [7, 11, 12, 14–18, 20, 23–25] and, as a rule of thumb, more disorder means slower growth. However, recent studies have shown that the growth law does not behave monotonically with increasing disorder in the two dimensional site or bond diluted Ising model [9]. In these systems, where a fraction  $D$  of sites or bonds is randomly removed from a regular lattice, one observes that, for sufficiently large  $D$ , more disorder produces faster growth. More precisely, starting from the pure case with  $D = 0$ , where the usual temperature-independent power-law  $L \sim t^{1/2}$  is obeyed, one enters a region with an asymptotic logarithmic behavior as soon as  $D > 0$ . However a temperature-dependent power-law growth is observed right at  $D = D_c = 1 - p_c$ , where  $p_c$  is the critical percolation density, thus leading to a non-monotonic dependence of the speed of growth upon the disorder strength  $D$ . This counterintuitive behavior has been interpreted in terms of the topology of the network of occupied sites or bonds [9, 10] with the temperature-dependent algebraic behavior associated to the fractal properties of the percolating network.

In this Article, by studying numerically the site-diluted Ising model (SDIM) and the bond diluted one (BDIM) in  $d = 3$  we find a non-monotonous dependence of  $L$  on disorder qualitatively similar to the two-dimensional case. This suggests that the relation between growth-law and topology might be a rather generic property, a fact that could provide new insights into the problem of phase-separation in disordered ferromagnets.

This paper is organized as follows. In Sec. II we describe the models, the SDIM and the BDIM, that will be considered and studied throughout this paper. In Sec. III we present an overview of the results in  $d = 2$  whereas numerical simulations of the  $d = 3$  models are discussed in Sec. IV. In Sec. V we conclude the paper with a final discussion of the results and of some open issues.

## II. THE DILUTED ISING MODEL

### A. The network

In the SDIM a network is prepared by generating configurations of occupied sites as in random percolation. On the sites of a square three-dimensional lattice there are independent random variables  $n_i$ , which take values  $n_i = 1$  (occupied site) with probability  $p$  and  $n_i = 0$  (empty site) with probability  $D = 1 - p$ . The substrate is formed by the set of occupied sites. Any couple of nearest-neighbour occupied sites is connected by a *bond*.

In the BDIM, instead, starting from a regular square three-dimensional lattice one removes bonds between nearest-neighbouring sites  $\langle ij \rangle$  at random with probability  $D$ . Specifically, an independent random variable  $J_{ij}$  is defined

on each couple of nearest sites, which takes values  $J_{ij} = 0$  with probability  $D$  (bond is absent) and  $J_{ij} = J_0$  with probability  $1 - D$  (bond is present).

For both models,  $D$  will be referred to as dilution. We now describe the geometrical structure of the network as  $D$  goes from high to low values. Recalling that the percolation threshold is  $p_c \simeq 0.3116$  and  $p_c \simeq 0.2488$  for site and bond percolation respectively, for  $D > D_c = 1 - p_c$ , the network is a patchwork of finite clusters of occupied sites (bonds) with a characteristic size that diverges at the threshold and a fractal dimension  $d_f \simeq 2.5$  [27]. The dilution range  $D > D_c$  will not be considered in this paper since, lacking an infinite cluster, perpetual coarsening cannot be sustained. At  $D_c$ , the size of the percolating cluster of sites (bonds) diverges. As  $D$  is lowered below  $D_c$ , the infinite cluster has a fractal geometry over distances up to a typical length  $\xi(D)$  that diverges at the threshold as

$$\xi(D) \sim (D_c - D)^{-\nu}, \quad (1)$$

with  $\nu \simeq 0.875$ , whereas it becomes compact over larger distances. Moreover, clusters of finite size are also present. The structure of the network described above holds in the range  $D_c \geq D \geq D^*$ , where  $D^*$  is a dilution value where

$$\xi(D^*) = a, \quad (2)$$

and  $a$  is a microscopic length, like the lattice spacing. For  $D < D^*$ , the infinite cluster is compact on any lengthscale and finite clusters are absent. The remaining far-apart vacancies inside this cluster are essentially single-site objects. Their average distance defines a new characteristic length

$$\lambda(D) = a(D^*/D)^{\frac{1}{d}}. \quad (3)$$

## B. Spin system

The diluted Ising model is described by the following Hamiltonian

$$H = - \sum_{\langle ij \rangle} K_{ij} \sigma_i \sigma_j. \quad (4)$$

Here  $\sigma_i = \pm 1$  are spins on the 3-d square lattice, and the couplings  $K_{ij}$  for the SDIM is chosen as  $K_{ij} = J_0 n_i n_j$ , where  $J_0$  is a constant, and  $n_i = 0$  or  $n_i = 1$  with probability  $D$  and  $1 - D$ , respectively. For the BDIM, instead,  $n_i = 1$  on all sites and  $K_{ij} = 0$  or  $K_{ij} = J_0$  with probability  $D$  and  $1 - D$ , respectively. Notice that, since  $J_0 > 0$ , the model is ferromagnetic.

## C. Equilibrium states

The equilibrium phase-diagram of the model is pictorially represented in Fig. 1. For  $D \leq D_c$ , at low enough temperature the system exhibits ferromagnetic order. In the  $(D, T)$  plane there is a critical line  $T_c(D)$ , which separates the paramagnetic from the ferromagnetic phase. The critical temperature  $T_c(D)$ , which in the following will be measured in units of  $k_B/J$ , where  $k_B$  is the Boltzmann constant, decreases from the pure value ( $T_c(0) \simeq 4.5$ ) as the dilution is increased and vanishes at  $D_c$  ( $T_c(D_c) = 0$ ).

## D. Time Evolution

Non-conserved dynamics[1, 2] is implemented by evolving the spins with single-spin-flip transition rates of the Glauber form

$$w(\sigma_i \rightarrow -\sigma_i) = \frac{1}{2} [1 - \sigma_i \tanh(H_i^W/T)]. \quad (5)$$

Here,  $H_i^W$  is the local Weiss field obtained by the sum

$$H_i^W = \sum_{j \in L_i} K_{ij} \sigma_j \quad (6)$$

over the set of nearest-neighbors  $L_i$  of  $i$ .

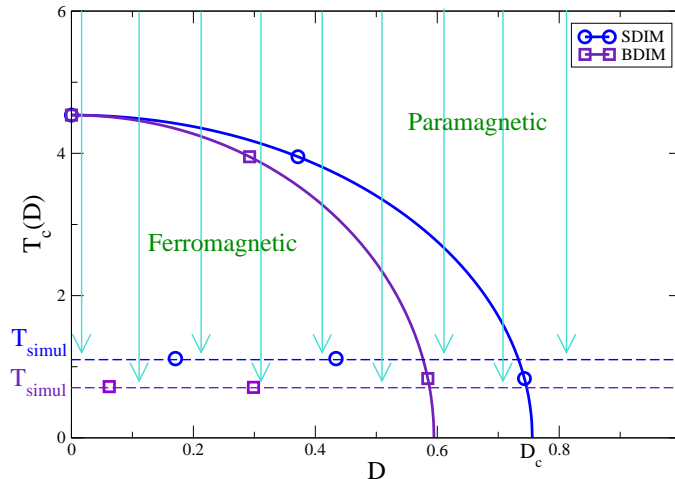


FIG. 1: (Color online) Pictorial representation of the equilibrium phase diagram of the diluted Ising model in  $d = 3$ . The bold blue line with circles and the bold indigo one with squares are the critical temperature  $T_c(D)$  of the SDIM and of the BDIM, respectively. The temperatures  $T = T_{simul}$  where simulations will be performed are marked with horizontal dashed lines, blue with circles for the SDIM and indigo with squares for the BDIM. Vertical arrows represent the quenching processes considered in the simulations.

The system is initially prepared in the infinite-temperature disordered state and, at the time  $t = 0$ , it is suddenly quenched to a finite temperature  $T$ . This temperature is set in the simulations to a value  $T_{simul} = 1.1$  for the SDIM and  $T_{simul} = 0.75$  for the BDIM. These values are chosen as a compromise: on the one hand we want to work in the limit of low-temperatures because the interplay between the two types of growth-law we are interested in is expected in the  $T \rightarrow 0$  limit [9]. On the other hand very low temperatures are useless in simulations for at least a couple of reasons. The first is that at very low temperatures pinning effects make the dynamics very slow. As a result the growing length  $L(t, D)$  does not vary appreciably in the time range accessed by the simulations and it is difficult to discriminate between different growth-laws. The second related reason is that at low temperatures the pinning centres produce a stop and go behavior of interfaces which, in turn, gives rise to an oscillatory behavior on top of the growth of  $L(t, D)$ . These oscillations prevent a reliable determination of the growth-law. A similar behavior is observed on fractal substrates [10, 13, 22].

In Sec. IV we will present the results of simulations of systems with different values of  $D$  in the range  $[0, D_c]$ . It must be noticed that, as discussed more detailedly in [9], for dilutions  $D = D_c$  or close to it the working temperature  $T = T_{simul}$  is necessarily larger than  $T_c(D)$ , see Fig. 1. Hence we are quenching above the critical temperature  $T_c(D_c) = 0$ , the system will eventually relax to a disordered state with a finite spin coherence length  $\xi_\sigma(T)$  (not to be confused with the substrate property  $\xi(D)$ ) and the growth of  $L(t, D)$  will eventually stop at  $t = t_{eq}(T)$  when  $L(t, D) \simeq \xi_\sigma(T)$ . In a preasymptotic stage with  $L(t, D) \ll \xi_\sigma(T)$  coarsening takes place and, since  $\xi_\sigma(T)$  diverges very fast for  $T \rightarrow 0$ , this can last for a very long time. The situation is similar to the one found in other ferromagnetic systems with  $T_c = 0$  as, for instance, the one-dimensional Ising model [28, 29]. We have checked that  $T_{simul}$  is sufficiently low as to never observe the equilibration of the system in the range of simulated times, and that the system keeps on coarsening at any simulated time.

### E. Observables

The observable quantity of interest in this paper is the typical domain size  $L(t, D)$ . For a model defined on a disconnected network, as it happens for  $D > D^*$ , phase ordering occurs independently on the various parts of the system and, correspondingly, different definitions of the growing length can be given. Following [9, 10], we determine this quantity from the inverse excess energy as

$$L(t, D) = [E(t, D) - E_\infty(D)]^{-1}, \quad (7)$$

where  $E(t, D) = \langle H \rangle$  is the energy at time  $t$ , the angular brackets denote a non-equilibrium ensemble average, taken over random initial conditions and over dynamical trajectories and disorder realizations, and  $E_\infty(D)$  is the energy

of the equilibrium state at the final temperature  $T$ . Eq. (7), which is often used to determine  $L(t, D)$  in non-diluted systems [1], has, in the present case, the further advantage that the disconnected finite parts of the substrate which are already ordered do not contribute to the computation of  $L(t, D)$ . Indeed each droplet is surrounded by empty sites in the SDIM or by null bonds in the BDIM and hence there is no excess energy associated with it when all spins are aligned, as discussed in [9, 10]. Using Eq.(7), then, one computes  $L(t, D)$  only on the regions where growth is active, which is the kind of information we are interested in.

### III. GROWTH LAW

#### A. Overview of the behaviour of the $2d$ -SDIM

In [9, 10] it was shown that the kinetic properties of the  $2d$ -SDIM and BDIM are due to the presence of three fixed points, in the sense of the renormalization group, existing on the  $D$  axis. The first fixed point is the trivial one of the pure system, located at  $D = 0$ , and is associated to the usual power-law growth  $L(t, 0) \sim t^{1/2}$ . The second one is the *percolative* fixed point located at  $D_c$  and is characterized by a temperature-dependent power-law growth

$$L(t, D_c) \sim t^{1/\zeta(T)}, \quad (8)$$

with  $\zeta(T) \geq 2$ . This new power-law growth is due to the fact that diluted sites act as pinning centres where interfaces get stucked unless an activation energy  $\Delta E$  is supplied by the thermal bath. According to the argument presented in [9, 10] this energy scales as  $\Delta E \sim A \ln L(t, D)$ . This is expected to be true for sufficiently low temperatures. Assuming an Arrhenius time  $t \sim \exp[\Delta E/(k_B T)]$  to exceed such energetic barriers one obtains Eq. (8) with an exponent

$$1/\zeta(T) = k_B T/A \quad (9)$$

proportional to the absolute temperature.

The two fixed points discussed above are repulsive, in the sense that as soon as  $D \neq 0$ , or  $D \neq D_c$  the asymptotic dynamics is governed by a different fixed point, located at  $D = D^*$  (roughly half way between  $D = 0$  and  $D = D_c$ ), to which a logarithmic increase of  $L(t, D^*)$  is associated. Due to these fixed point structure, if the system is prepared with an intermediate dilution between  $D = 0$  and  $D^*$  (or equivalently between  $D^*$  and  $D_c$ ) a crossover pattern is observed at a certain time  $t_{cross}(T, D)$  from an initial transient regime governed by the nearest unstable fixed point ( $D = 0$  or  $D_c$  respectively), with a power-law increase of the domains size, to a late regime controlled by the attractive point at  $D^*$ , characterized by a logarithmic  $L(t, D)$ . The crossover phenomenon occurs when  $L(t, D)$  reaches the typical size associated to dilution, which is either  $\lambda(D)$  or  $\xi(D)$  depending on  $0 < D < D^*$  or  $D^* < D < D_c$ . Given that both  $\lambda$  and  $\xi$  decrease approaching  $D^*$  (Eqs. (1,3)), the slowest possible growth, namely the one where  $t_{cross}(T, D)$  is smaller, is obtained at  $D = D^*$ . Therefore by comparing  $L(t, D)$  for different values of  $D$  one finds a non-monotonous behavior: The growth slows down in going from  $D = 0$  to  $D = D^*$  and then speeds up again when  $D$  is further increased from  $D = D^*$  up to  $D = D_c$ . This can represent a practical tool to identify  $D^*$ .

In the next section we will show that a similar structure is observed also in  $3d$ .

### IV. NUMERICAL RESULTS

#### 1. Simulation details

The details of the simulations are as follows. We have considered a three-dimensional square lattice system of  $N = \mathcal{L}^2$  sites, with  $\mathcal{L} = 240$  for the SDIM and  $\mathcal{L} = 150$  for the BDIM. We have checked that, with this choice, no finite-size effects can be detected in the time-regime accessed by the simulations. For every choice of the parameters, we have performed a certain number (in the range 10-100) of independent runs with different initial conditions, disorder realizations and thermal histories in order to populate the non-equilibrium ensemble needed to extract average quantities.

To speed up the simulations we have used a modified dynamics where spin flips in the bulk of domains, namely those aligned with all the nearest neighbors, are prevented. This modified dynamics does not alter the behavior of the quantities we are interested in, as has been tested in the  $2d$  version of the models and in a large number of different cases [30]. We have checked that this is also true in the present study.

## 2. 3d results: SDIM

Let us start by considering the SDIM. The time dependence of  $L(t, D)$ , for various dilution values, is plotted in Fig. 2 for the 3d-SDIM. Notice that we plot  $L(t, D)/L(15, D)$  in order to normalize the curves at the microscopic time  $t_{micro} \simeq 15$  when the late-stage scaling regime is entered.

In the pure case the asymptotic power-law  $L(t, 0) \sim t^{1/2}$  is expected. In the relatively small range of simulated times we measure a somewhat smaller exponent (in the last decade a best fit procedure yields  $1/z \simeq 0.46$ , as already reported in [31, 32], because the convergence to the true asymptotic behavior is very slow, as explained in [32]. Indeed the observed *effective* exponent  $1/z$  appears to increase with time. However here we are mainly interested in the non-monotonic behavior of the speed of growth for which an accurate estimate of  $z$  is not necessary. In fact, it is clearly observed that, by increasing  $D$ , the growth law becomes slower and slower up to a certain value of  $D \simeq 0.5$  that, following [9], we identify with  $D^*$ . For  $D > D^*$  growth becomes faster upon increasing  $D$  up to  $D_c$ . This behavior results in a non-monotonic  $D$ -dependence of  $L(t, D)$ , at fixed time  $t$ . This can be clearly appreciated in the inset of Fig. 2 where the behavior of the effective exponent obtained by fitting the data for various  $D$  with a power-law (regardless of the fact that the actual growth-law might not be power-law) in the time-range  $t \geq 5000$ .

Having established the non-monotonous dependence of the speed of growth on  $D$ , we make some comments on the form of the growth-law. At the dilution  $D = D^*$  we observe a downwards banding of  $L(t, D)$  which indicates that the growth is slower than algebraic, suggesting in this case a logarithmic law. We recall that a form  $L(t, D) \simeq (\ln t)^{1/\phi}$  was predicted in a model with bond disorder in [21], which, however, due its slow character has never been accurately demonstrated, to the best of our knowledge, even in the less numerically demanding 2d cases. Clearly in this 3d case the task is much more demanding, and the time range accessible in the simulations is not sufficient for a precise determination of the analytical form of the growth-law.

For  $D = D_c$ , on the other hand, the behavior of  $L(t, D_c)$  is well fitted, as expected, by a power-law  $L(t, D_c) \simeq t^{1/\zeta(T)}$ , with  $1/\zeta(T_{simul}) \simeq 0.41$ . According to the discussion of Sec. III A, this behavior is expected irrespective of the quenching temperature (but with a different temperature-dependent exponent  $\zeta$ ), provided it is sufficiently low. In order to check this we have performed a series of simulations by fixing  $D = D_c$  and changing  $T_{simul}$ . The behavior of  $L(t, D)$  in these cases is shown in Fig. 3. The data are consistent with power-laws for any choice of  $T_{simul}$ . Notice however that for very small  $T_{simul}$  the power-law is decorated by a sort of log-time periodic oscillation. The exponent  $1/\zeta(T)$ , obtained by fitting all the curves in the last decade (for  $T = 0.5$  we use two decades in order to smear out the oscillation), is plotted in the inset. According to Eq. (9), one finds a linear behavior at sufficiently low temperatures. Fitting this curve we obtain  $A \simeq 0.36$  (Eq.(9)). Notice that for large values of the temperature this linear behavior breaks down, due to the constraint  $1/\zeta(T) \leq 1/2$  since it is impossible to grow faster than in the pure case.

## 3. 3d results: BDIM

In order to check the generality of the behaviors observed in the SDIM we have performed a series of simulations also for the 3d-BDIM. Unfortunately, for this model it is not possible to find a region of sufficiently low temperatures to be considered representative of the  $T \rightarrow 0$  limit, as discussed in Sec. II D, but high enough to eliminate the stop and go behavior of the interfaces, which is responsible for the oscillatory character of  $L(t, D)$ . We have explored several values of  $T_{simul} < 1$ , and in all cases we observe a non-monotonic behavior of  $L(t, D)$  as  $D$  is varied. In Fig. (4) we plot results for  $T_{simul} = 0.75$ . For quenches at this temperature oscillations are clearly evident ruling out the possibility to make any statement on the form of the growth-law (whether logarithmic or power-law). Despite this, the non monotonic behavior of  $L(t, D)$  as  $D$  is varied at fixed  $t$  is quite evident from Fig. 4. Starting from the pure case  $D = 0$ , where a fast growth is observed (although much slower than the asymptotic expected behavior  $L(t, 0) \sim t^{1/2}$ , due to the long-lasting pre-asymptotic corrections discussed above) the growth gets slower as  $D$  is increased up to  $D = D^* \simeq 0.5$ , and then speeds up again until  $D_c$  is reached. This shows that the non-monotonicity of the speed of growth as disorder is increased is a general property of diluted system, irrespective of dimension and of the kind of dilution. This suggests that an interpretation based on the presence of three fixed points, the pure one and those at  $D^*$  and  $D_c$ , and the attractive/repulsive nature of such fixed points, can be appropriated quite generally.

## V. CONCLUSIONS

In this paper we have studied the diluted Ising model in three dimensions. The aim of the paper was to show the generality of the phase-ordering behavior previously observed in the 2d-SDIM and 2d-BDIM, where it was first shown [9, 10] the non-monotonous dependence of the speed of growth on the amount of disorder, a fact that was interpreted as

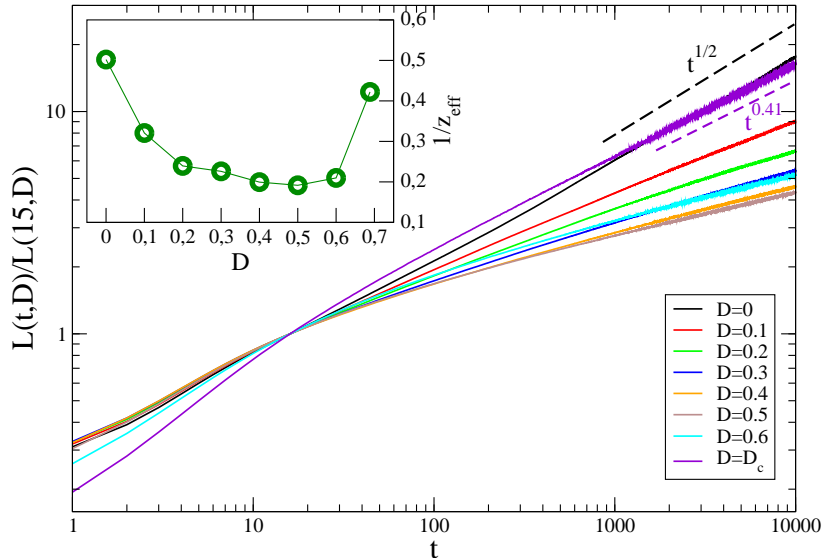


FIG. 2: (Color online) The behavior of the typical length  $L(t,D)/L(15,D)$  after a quench to  $T = T_{simul}$  is shown for the SDIM for several dilutions  $D$  (see legend) in a double logarithmic plot. The dashed-black line is the pure growth-law  $L(t,0) \sim t^{1/2}$  and the dashed-violet one is the power-law  $L(t,D_c) \sim t^{0.41}$ . In the inset the effective exponent  $1/z_{eff}$  (see text) is plotted against  $D$ .

due to the close relation between the coarsening properties and some topological features of the network in disordered magnets. In order to do that we have considered three-dimensional systems.

Our results show that the pattern of behavior observed in these models is analogous to the one found in the 2d SDIM and RBIM, and henceforth an analogous interpretation can be given. In the pure system phase-ordering occurs without activation energy by a smooth curvature-driven displacement of interfaces, leading to the well known growth-law  $L(t,0) \sim t^{1/2}$ . The situation changes radically as soon as disorder is introduced, because inhomogeneities pin the interfaces in energy minima and thermal activation is required to proceed. In [9] an argument was developed leading to the conjecture that the  $L(t,D)$ -dependence of the pinning barriers changes when passing from  $D < D_c$  to  $D = D_c$ , due to a radically different large-scale topology of the network which turns from a compact to a fractal object. This implies also a different growth-law, logarithmic for  $D < D_c$  vs power-law  $L(t,D_c) \sim t^{1/\zeta(T)}$  right at  $D_c$ . In a renormalization-group language this features can be accommodated in a framework with three fixed points, located at  $D = 0$ ,  $D = D^*$  and  $D = D_c$ . Accordingly, a crossover phenomenon is observed where, for any  $0 < D < D_c$ ,  $L(t,D)$  changes from an early behavior associated to the nearest repulsive fixed point to the asymptotic logarithmic law. This gives rise to the non-monotonic behavior of  $L(t,D)$  as  $D$  is varied keeping  $t$  fixed.

The presented numerical study suggests that the pattern of behaviors observed in [9, 10] is quite a general feature of ferromagnetic disordered systems. Indeed we find that the non-monotonic behavior of  $L(t,D)$  is observed also in 3d systems. Our results also indicate that, at least for the SDIM,  $L(t,D_c)$  exhibits a power law growth with a growth exponent  $\zeta(t)$  inversely proportional to the temperature. The growth law becomes slower as  $D$  is decreased to  $D^*$ , even if our data do not allow the precise determination of a logarithmic growth for  $L(t,D^*)$ . It would be an interesting line of research to investigate if a similar structure underlies also the kinetics of other disordered systems such as, for instance, Ising models with random fields.

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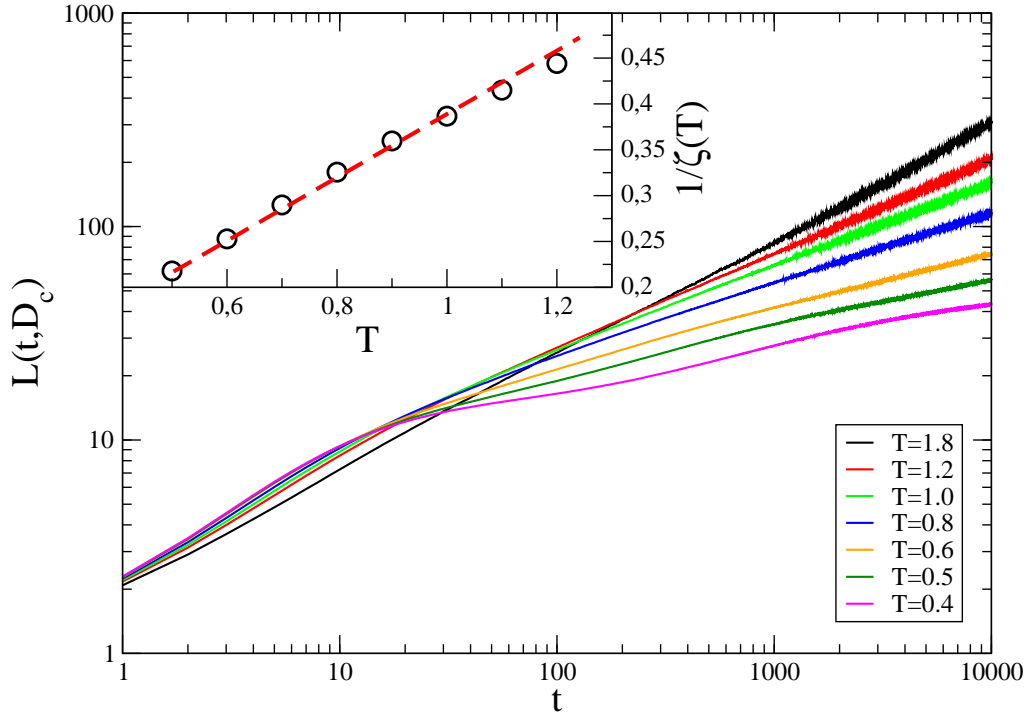


FIG. 3: (Color online) The behavior of the typical length  $L(t, D_c)$  after a quench to different temperatures  $T_{simul}$  (see key) of the SDIM is shown in a double logarithmic plot. In the inset we plot the best fit exponent  $1/\zeta(T)$  as function of  $T$ . The red dashed line is the theoretical value (Eq.(9)) with  $A = 0.36$ .

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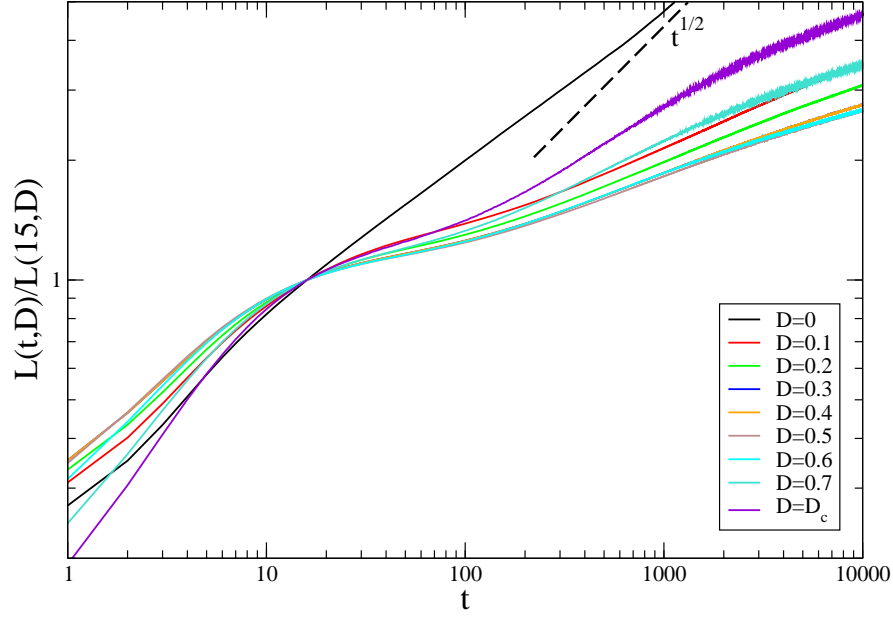


FIG. 4: (Color online) The behavior of the typical length  $L(t,D)/L(15,D)$  after a quench to  $T = T_{simul}$  is shown for the BDIM for several dilutions  $D$  (see legend) in a double logarithmic plot. The dashed-black line is pure growth-law  $L(t,0) \sim t^{1/2}$ .

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